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BOOK OF ABSTRACTS

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Influence of moments of inertia of molecules on the structure of shocks in molecular liquids

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The present paper is the last part of the series of our papers on the structure of shock waves in dense media. The main results obtained till now are:
- The length scale, most appropriate for measuring the thickness of a shock wave in dense medium, is the average distance between the centers of the neighbouring molecules [1].
- For a dense, monoatomic, noble gas, argon, the "density shock thickness" related to the average distance between molecules decreases with increasing density, which is mainly due to decrease of the shock amplitude at approximately the same density gradient [1].
- For polar liquids (water, hydrogen sulfide, hydrogen fluoride) the presence of electric charges does not seem to influence noticeably the density gradient inside the shock. It may, however, influence compressibility of the medium, manifesting itself in the change of shock amplitude and, as a result, influence the shock thickness. This can be noticed for strongly polar liquids: water and hydrogen fluoride [2].
- For a complex molecular medium, sulfur hexafluoride, the shock thickness in the liquid phase related to the mean distance between the molecules is larger than that in the rarefied gas phase, related to the mean free path. This is opposite to the result for the simple substance – argon. The possible reason is that the molecules of sulfur hexafluoride, having large moments of inertia, in the liquid phase stay constantly in close contact and therefore probably need more time for excitation of rotational degrees of freedom which, in turn, may increase the shock thickness [3].

To learn more about influence of the moments of inertia, in this paper we compare the structures of shock waves in non-polar liquids, having molecules of similar shape but differ- ent moments of inertia: methane (CH_4) – tetrafluoromethane (CF_4) – carbon tetrachloride (CCl_4).

The presented results were obtained with the standard Molecular Dynamics technique. The molecules were assumed to consist of atoms rigidly connected; each atom interacted with atoms of other molecules through the Lennard - Jones potential. The shock was generated when a mass of liquid, moving with high velocity, collided with a plane wall perpendicular to the direction of motion.

References

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